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Computing third-order models of effective material behavior for polydisperse particulate composites using well-resolved higher order statistical descriptors

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ABSTRACT

Accurately characterizing and modeling random heterogeneous media such as energetic materials, geomaterials, and other granular systems is essential to improving design and developing new material formulations. The focus of this study is to estimate and bound the effective thermo-mechanical behavior using well-resolved statistical descriptions of polydisperse particulate systems to develop microstructure–statistics–property relations. In past study related to bounding effective material properties using variational methods that incorporate statistical information about the microstructure, assumptions are often made about the configuration (isotropy, ellipsoidal symmetry, monodisperse spheres) to simplify analysis. However, real systems are often not composed according to these microstructural assumptions. When these assumptions are not valid, complex integrals containing the product of the Green's function solution and higher-order statistical functions cannot be simplified analytically and must be evaluated numerically. In our prior study [1,2], a second order model with perfect interface behavior between constituents has been considered when computing bounds of anisotropic effective thermo-mechanical properties. However, it is known that incorporating higher order statistical information will increase the accuracy of these bounds. In this presentation, we will focus on computing third-order bounds and estimates of effective thermo-mechanical properties for polydisperse particulate systems only assuming statistical isotropy [3]. This study relies on parallel adaptive methods rooted in computational mechanics for efficiently representing statistical functions arising in the third-order models for effective material behavior. These computational methods are verified for systems of overlapping and impenetrable monodisperse spheres, and we show up to 46% improvement over state of the art techniques and excellent agreement with simulation data. We demonstrate the extensibility of these methods to microstructures with polydisperse particles of arbitrary shape, which are classes of systems earlier unstudied. In particular, we present results for random systems of ellipsoids and crystals for a large range of volume fractions.

REFERENCES

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